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Difference Methods on a Digital Computer for Laplacian Boundary Value and Eigenvalue Problems

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Reprinted from

COMMUNICATIONS ON PURE AND APPLIED MATHEMATICS Volume IX, No. 3

August, 1956

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Difference Methods on a Digital Computer for Laplacian Boundary Value and Eigenvalue Problems*

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1. Finite Difference Approximations

We begin with

DEFINITION 1. A simple closed curve Γ : x(s)+iy(s) $(0 \le s \le s_t)$ is said to be piecewise analytic if x(s) and y(s) are real analytic functions of the arc length s of Γ in each of a finite number t of closed intervals $0 = s_0 \le s \le s_1$, $s_1 \le s \le s_2$, \cdots , $s_{t-1} \le s \le s_t$.

Let the open region R of the x, y-plane have a boundary C which is the union of a finite number of piecewise analytic simple closed curves. For real-valued functions u = u(x, y) defined on $R \cup C$, denote by Δu the Laplacian $u_{xx} + u_{yy}$. In numerical computations R, C, u, and Δu are frequently replaced by corresponding quantities associated with a finite difference network. These may be introduced as follows (see [1] for a similar treatment):

For a given mesh constant h > 0 let a net consist of the lines $x = \mu h$, y = vh, μ , $\nu = 0, \pm 1, \pm 2, \cdots$. The points $(\mu h, \nu h)$ are called nodes. The M nodes which are within R form the net region R_h , assumed to be connectable by line segments of the net within R. A point $(\mu h, \nu h)$ of R_h is said to be a regular interior point if each of the four neighboring nodes $(\mu h \pm h, \nu h \pm h)$ is in $R \cup C$. All other points of R_h are called irregular interior points. Certain points P of R_h have some number p ($1 \le p \le 4$) of neighboring nodes P_1 , \cdots , P_n not in the open region R. For any such point P, let P0 denote the closed segment of the net joining P1 to P1. For each P2, the point of P3 denote the net joints will be called a boundary point of the net. The set of boundary points will be denoted by P3. Some points of P4 may be nodes, but each irregular interior point of P4 has one or more neighboring points in P3 which are not nodes. (The definition of P3 given in [2], although intended to be the same, is not precise.)

^{*}The research leading to this paper was sponsored jointly by the Office of Naval Research, project NR-044-144, and the Office of Ordnance Research, project TB2-0001(1210).

Corresponding to u, defined on $R \cup C$, is a real-valued net-function $u=u_h$ defined on $R_h \cup C_h$. Corresponding to Δu is $\Delta^{(h)}u$ defined as follows. For each point P:(x,y) of R_h , let the neighboring points of $R_h \cup C_h$ be denoted by $(x+h_E, y)$, $(x, y+h_N)$, $(x-h_W, y)$, and $(x, y-h_S)$, where each of the h's is positive ($E \sim$ "east"; $N \sim$ "north", etc.). Let $b_E = h_E/h$, $b_N = h_N/h$, etc. For regular interior points $b_E = b_N = \cdots = 1$. Let $u(x, y) = u_P$, $u(x+h_E, y) = u_E$, $u(x, y+h_N) = u_N$, etc.

Define the residual r_P at P by

(1)
$$r_P = \frac{u_E}{b_E(b_E + b_W)B} + \frac{u_W}{b_W(b_E + b_W)B} + \frac{u_N}{b_N(b_N + b_S)B} + \frac{u_S}{b_S(b_N + b_S)B} - 4u_P$$
, where

$$B = \frac{1}{4b_N b_S} + \frac{1}{4b_E b_S}.$$

Then

$$\Delta^{(h)}u=r_p/h^2.$$

(The definition of $\Delta^{(h)}u$ in [2] differs by the factor 2B.) In case P is a regular interior point, (1) reduces to the usual formula

(3)
$$r_P = u_E + u_W + u_N + u_S - 4u_P$$

When there are irregular interior points, the operator $\Delta^{(h)}$ is not self-adjoint over R_h . For treating the eigenvalue problem it is often more convenient to deal with the self-adjoint part of $\Delta^{(h)}$, denoted here and in [2] by Δ_h .

2. Asymptotic Inequalities for All Eigenvalues

For the operator Δ , the eigenvalue problem

(4)
$$\Delta u + \lambda u = 0 \quad \text{in } R, \\ u = 0 \quad \text{on } C$$

is known to have an infinite sequence of linearly independent eigenfunctions $u^{(k)}$ and corresponding eigenvalues $\lambda^{(k)}$, numbered so that

$$(5) \qquad 0 < \lambda^{(1)} < \lambda^{(2)} \leq \lambda^{(3)} \leq \cdots$$

Similarly, the eigenvalue problem

(6)
$$\Delta_h u + \lambda_h u = 0 \quad \text{on } R_h,$$

$$u = 0 \quad \text{on } C_h$$

has a finite sequence of linearly independent eigenfunctions $u_h^{(k)}$ and eigenvalues $\lambda_{h}^{(k)}$, where

$$0<\lambda_h^{(1)}<\lambda_h^{(2)}\leq\lambda_h^{(3)}\leq\cdots\leq\lambda_h^{(M)}.$$

(Recall that M is the number of points of R_h .)

For rectangles whose sides are lines of the net, it is well known that

(7)
$$\lambda_{h}^{(k)} < \lambda_{h}^{(k)}, \qquad k = 1, \dots, M;$$

see also below. Since for general regions R close lower bounds for the $\lambda^{(k)}$ are not easily found, the author has been investigating [3, 5a, 2, 4] whether (7) might also hold for other regions.

Suppose one deals with a polygonal region R which is a finite union of squares and half-squares of a net of mesh constant 2h. Then R_{2h} has no irregular interior points, and neither does R_h , obtained by refining the net. At any point (x, y) of R_{2h} ,

$$\Delta_{2h}u = \Delta_h u + \frac{1}{4}h^2 L_h u,$$

where $L_h u = h^{-4} \{u_{xx\bar{x}\bar{x}} + u_{yy\bar{y}\bar{y}}\}$. Here

$$u_{xx\bar{z}\bar{x}} = u(x-2h,y) - 4u(x-h,y) + 6u(x,y) - 4u(x+h,y) + u(x+2h,y),$$

and $u_{\nu\nu\bar{\nu}\bar{\nu}}$ is defined analogously. Following the idea [3] of putting the fundamental eigenfunction $u_{h} = u_{h}^{(1)}$ of the problem for R_{h} into the minimization problem for R_{2h} , one finds that

(9)
$$\lambda_{2h}^{(1)} \leq \lambda_{h}^{(1)} - \frac{1}{4}h^{2} \left(\sum_{(2h)} u_{h} L_{h} u_{h} \right) \left(\sum_{(2h)} u_{h}^{2} \right)^{-1},$$

where $\sum_{(2h)}$ denotes a sum over the points of R_{2h} . Hence whenever

$$\sum_{(2h)} u_h L_h u_h > 0$$

it follows that

$$\lambda_{2k}^{(1)} < \lambda_k^{(1)}.$$

If (11) should hold also for h replaced by h/2, h/4, h/8, \cdots , it would then follow that $\lambda_h^{(1)} < \lambda^{(1)}$, since the methods of [5] show that $\lambda_h^{(1)} \to \lambda^{(1)}$, as $h \to 0$.

Recent computation with SWAC (see Section 4 below) for the L-shaped region of [3] shows that (11) fails for h=1/16. Hence (10) is not true for all polygonal regions of the type considered here. I conjecture, however, that (10) holds for any convex R which is the union of squares and half-squares of the net.

Lacking a proof of this conjecture, the author proved [3] an asymptotic form of (7) for k=1, and in [5a] and [2] generalized it to include certain regions with curved boundaries (the case k=1 of Theorem 2 below). Thus, under the hypotheses of Theorem 2 below, the desired inequality (7) has already been proved for the first eigenvalue, though only for sufficiently small h. Less delicate inequalities of type $\lambda_h^{(1)} < \lambda^{(1)}$, valid for all h, have since been found by Weinberger [6, 7] and Hersch [8] without such stringent hypotheses on R, by allowing R_h to correspond to a region a little larger than

R. Assuming x(s), y(s) defining Γ to be seven times continuously differentiable, Saul'ev [8a] has recently found inequalities of the type $|\lambda_h^{(k)} - \lambda^{(k)}| = O(h^{2-\epsilon})$, as $h \to 0$.

During the 1955 Berkeley Conference for Partial Differential Equations, at which this paper was presented, the author completed an extension of the results of [2] to all eigenvalues of Δ and Δ_h . This has been abstracted in [4], and will now be summarized. Let τ be the angle between the x-axis and the positive direction of the tangent to C. For any function v, let v_n denote the inner normal derivative of v on C. For any two functions v, w, define an inner product (v, w) by the formula

$$12(v, w) = \iint_{R} (v_{xx}w_{xx} + v_{yy}w_{yy}) dx dy + \int_{C} v_{n}w_{n} \sin^{2} 2\tau d\tau.$$

Let the infinite symmetric matrix D have elements $d_{ij} = (u^{(i)}, u^{(j)})$, $i, j = 1, 2, \dots$, where $u^{(k)}$ is an eigenfunction of (4) belonging to $\lambda^{(k)}$, normalized so that $\iint_R (u^{(k)})^2 dx dy = 1$. Corresponding to an m-fold multiple eigenvalue of Δ , we are to take m linearly independent functions $u^{(k)}$.

Define a sequence of real numbers $\gamma^{(k)}$, $k=1,2,\cdots$, as follows. If $\lambda^{(k)}$ is a simple eigenvalue of (4), take $\gamma^{(k)}=d_{kk}$. If $\lambda^{(k)}=\lambda^{(k+1)}=\cdots=\lambda^{(k+m-1)}$ is an m-fold multiple eigenvalue of (4), then define $\gamma^{(k)} \geq \gamma^{(k+1)} \geq \cdots \geq \gamma^{(k+m-1)}$ to be the m (real) eigenvalues of (d_{ij}) , $i,j=k,\cdots,k+m-1$, the corresponding m-rowed principal minor of D.

DEFINITION 2. A region R bounded by a finite number of piecewise analytic curves is said to have strictly convex corners if, at any point $x(s_j)$ + $iy(s_j)$ where distinct analytic curves meet (see Definition 1), the interior angle is less than π (equality not permitted).

THEOREM 1. Let R, an open region with strictly convex corners, be bounded by C, the union of a finite number of piecewise analytic, simple closed curves. Define h, $\lambda_h^{(k)}$, $\lambda_h^{(k)}$, $\gamma^{(k)}$ as above. Then for $k = 1, 2, \cdots$ one has $-\infty < \gamma^{(k)} < \infty$ and, as $h \to 0$,

(12)
$$\lambda_h^{(k)} \leq \lambda^{(k)} - \gamma^{(k)} h^2 + o(h^2).$$

A proof of Theorem 1 will appear in a later paper. If R is also convex, then C is a simple closed curve with $d\tau \ge 0$, and D is therefore a Gramian matrix. Hence all $\gamma^{(k)} > 0$, and we have the following corollary to Theorem 1:

THEOREM 2. Let R, a convex open region with strictly convex corners, be bounded by C, a piecewise analytic, simple closed curve. Then, with the above notation, $0 < \gamma^{(k)} < \infty$, and for each $k = 1, 2, \cdots$ there exists $h_0(k) > 0$ such that $\lambda_h^{(k)} < \lambda^{(k)}$ if $h \leq h_0(k)$.

The case k = 1 of Theorems 1 and 2 is the result proved in [2]. (In Theorem 1 of [2] the assumption that R be simply connected was never used. Note: The proof of Lemma 1 in [2] is incorrect.)

As an asymptotic result Theorem 1 is the best possible, in the following sense. For a rectangle R of sides π/p , π/q , the relation (12) is actually an equality for all k, up to the term $o(h^2)$. For, corresponding to the eigenfunction $u^{(m,n)} = \sin mpx \sin nqy$ of both (4) and (6) (it is convenient here to use a double superscript m, n instead of the single superscript k), one has

$$\lambda^{(m,n)} = (mp)^2 + (nq)^2;$$

and, as $h \to 0$ over values of h for which R is a union of squares of the net,

(13)
$$\lambda_h^{(m,n)} = \frac{\sin^2(mph/2) + \sin^2(nqh/2)}{(h/2)^2}$$

$$= \lambda^{(m,n)} - \frac{(mp)^4 + (nq)^4}{12} h^2 + o(h^2)$$

$$= \lambda^{(m,n)} - (u^{(m,n)}, u^{(m,n)})h^2/12 + o(h^2).$$

Since $(u^{(m,n)}, u^{(\mu,\nu)}) = 0$ unless $|m-\mu| + |n-\nu| = 0$, one has $\gamma^{(m,n)} = (u^{(m,n)}, u^{(m,n)})/12$, even for multiple eigenvalues. Hence (13) shows that (12) is an equality for the rectangle R, up to the term $o(h^2)$.

3. Solving the Difference Equations on a Machine

Let us first consider solving the Dirichlet difference problem

(14a)
$$\Delta^{(h)}u=0 \quad \text{on } R_h,$$

(14b)
$$u = \text{prescribed function on } C_h$$

on an automatic digital computer. Assume there are no irregular interior points of R_h , so that (14a) is equivalent to

(14c)
$$r_P = u_E + u_N + u_W + u_S - 4u_P = 0$$
 on R_h

To solve the system of M equations (14c) in the unknown values of u at the M points of R_h , iterative methods are usually preferable to elimination methods, because of their simplicity. The successive overrelaxation process of [10] and [9] has proved very successful. In it the points of R_h are repeatedly scanned in a cyclic order. In its turn, at each point P of R_h the value u_P is immediately replaced by a new value u_P' ,

$$u_P' = u_P + \frac{1}{4}\beta r_P,$$

where β ($1 \le \beta < 2$) is a parameter to be discussed below. Using the new value of u_P , one goes on to the next point of R_h , and so on. For $\beta = 1$ this

is the *Liebmann process* [11], in which $u_P' = \frac{1}{4}(u_E + u_N + u_W + u_S)$. Any reasonable initial values $u_{\beta}^{(0)}$ of the function u over R_h will suffice, and one may take all $u_{\beta}^{(0)} = 0$.

Let $u_{\beta}^{(k)}$ be the result of k sweeps through R_k with successive overrelaxation. Let $u^{(\infty)}$ be the exact solution of (14); define the error $e_{\beta}^{(k)} = u_{\beta}^{(k)} - u^{(\infty)}$. Since the solution process is linear, one knows that

$$e_{\beta}^{(k)} = H_{\beta}^{k} e_{\beta}^{(0)}$$
,

where H_{β} is a certain linear transformation of R_{λ} into itself. The convergence of $e_{\beta}^{(k)}$ to 0, as $k \to \infty$, depends on the maximum modulus of the eigenvalues $\lambda_i(H_{\beta})$ of H_{β} . For the Dirichlet problem it is known [9] that $|\lambda_i(H_{\beta})| < 1$ (all i, $0 < \beta < 2$), so that successive overrelaxation ($1 \le \beta < 2$) always converges. The ultimate speed of convergence depends on $\max_i |\lambda_i(H_{\beta})|$. Now, for any single step (15), to choose $\beta = 1$ is the best tactic, in the sense that the negative definite error function $\sum_{R_{\lambda}} e \Delta^{(\lambda)} e$ is brought as close to the desired value 0 as is possible in the one step, by choosing $\beta = 1$ in (15). However, hand computers have long observed [12] that certain choices $\beta > 1$ apparently represent a better strategy than $\beta = 1$, in the sense that $e_{\beta}^{(k)} \to 0$ faster asymptotically, as $k \to \infty$. (Related ideas of strategy and tactics for other linear processes will be found in [13].) In [10] and [9] the matter of a best strategy is settled by showing how to pick the unique β_0 for which $\max_i |\lambda_i(H_{\beta})|$ is minimized. Indeed,

$$\beta_0 = \frac{2}{1+\sqrt{1-\sigma}},$$

where

(17)
$$\sigma = \max_{i} |\lambda_{i}(H_{1})|.$$

The number σ is easily approximated by setting $\beta=1$ and estimating the asymptotic value of $||e_1^{(k+1)}||/||e_1^{(k)}||$, as $k\to\infty$, where $||\cdot||$ denotes some convenient norm function. When $\beta=\beta_0$, all the $|\lambda_i(H_\beta)|$, $i=1,\cdots,M$, turn out to be equal, so that the manner of approach of $||e_{\beta_0}^{(k)}||$ to 0 is utterly unpredictable.

When R has a curvilinear boundary C, the theory of [9] still holds, and the successive overrelaxation method is just as attractive. One simply replaces the formula (3) for r_P at irregular interior points P of R_A by the formula (1).

For the eigenvalue problem (6) successive overrelaxation is readily adaptable to getting $\lambda_{\lambda}^{(1)}$ and its associated eigenvector $u_{\lambda}^{(1)}$. One uses a trial value λ for $\lambda_{\lambda}^{(1)}$, and solves the system

(18)
$$(\Delta_h + \lambda I)u = 0 \quad \text{on } R_h,$$

$$u = 0 \quad \text{on } C_h$$

by successive overrelaxation starting with some nonzero vector $u_{\beta}^{(0)}$. For the residual, assuming that R_h has only regular interior points (so that $\Delta_h \equiv \Delta^{(h)}$), one uses

(19)
$$r_{P} = u_{E} + u_{N} + u_{W} + u_{S} - 4u_{P} + \lambda u_{P}$$

in (15). If λ were exactly equal to $\lambda_h^{(1)}$, the iterates $u_{\beta}^{(k)}$ would stay roughly in the affine subspace S (of M-dimensional space) which is orthogonal to $u_h^{(1)}$ and passes through $u_{\beta}^{(0)}$. Apart from an exceptional set of $u_{\beta}^{(0)}$ of zero measure, one would always have $u_{\beta}^{(k)} \to \alpha u_h^{(1)}$, as $k \to \infty$, where α is some nonzero number depending on $u_{\beta}^{(0)}$. If λ is near $\lambda_h^{(1)}$ but not equal to it, one finds that $u_{\beta}^{(k)}$ moves asymptotically into the line $\alpha u_h^{(1)}$ while converging to 0 or ∞ . An improved value of λ is then obtainable from the Rayleigh quotient $\varrho_h(u_{\beta}^{(k)})$, where

(20)
$$\varrho_h(v) = -\left(\sum_{R_h} v \Delta_h v\right) \left(\sum_{R_h} v^2\right)^{-1}.$$

One then uses the better λ in (19), and alternates a few steps of successive overrelaxation with the Rayleigh quotient calculation, until a satisfactory $\alpha u_h^{(1)}$ is obtained.

For getting $\lambda_h^{(k)}$ and $u_h^{(k)}$ (k > 1), the idea of solving (18) with λ near $\lambda_h^{(k)}$ is undoubtedly still a good one, but successive overrelaxation no longer converges, because $\Delta_h + \lambda_h^{(k)} I$ is not semidefinite for k > 1. A simple iteration which can solve indefinite systems must be substituted—perhaps that of Kaczmarz [14].

4. SWAC Codes

SWAC is an electronic digital computer built by the National Bureau of Standards, but now owned by the Department of Defense and loaned to the University of California, Los Angeles, for research in numerical analysis. It is a three or four address machine with a Williams tube memory of 256 words; each word consists of 36 binary digits and a sign. Add time is .000064 second; multiplication time is slightly less than six add times. An auxiliary magnetic drum memory holds 4096 words in 128 channels of 32 words each (increased to 8192 words in late 1955). One can transfer a block of up to 32 words between the drum and the Williams tube memory in .017 second. For substantial problems, computing time is measured in hours, while coding time is measured in weeks.

In connection with the author's graduate seminar on numerical methods for elliptic partial differential equations, held in the spring of 1955, a few general codes were prepared following the methods of Section 3 above.

In all these codes the net region R_h is represented by a subset of the

32 by 128 rectangular array of cells on SWAC's magnetic drum. Parameters indicate the smallest rectangle in which R_h is contained. In all the codes the data in successive drum channels are brought to the Williams tube memory for the relaxation process, and the improved values are sent back when they are no longer needed.

The author's basic Code 60 solves Dirichlet's problem for the operator $\Delta^{(h)} \equiv \Delta_h$ for a region with no irregular interior points. Here C_h consists solely of nodes of the net, and can thus also be represented by cells of the drum. Points of R_h have a 0 in the most significant binary digit. Points not in R_h are tagged with a 1 in the same digit, and can be an arbitrary subset of the 32 by 128 rectangular array. Code 60 assumes that the values of u have been placed in the drum cells representing C_h , in digits less significant than the first (which is assumed to be tagged with a 1, as stated above). It performs successive overrelaxation at all points of R_h , leaving all other values of u unchanged. The overrelaxation factor β defined in Section 3 can be modified at will by the SWAC operator. (It is fun for the operator to participate in the solution. Having the operator manage β , while SWAC manages all other numbers, seems a satisfactory division of labor!) The error measure used, denoted by $||e_{\beta}^{(k)}||$, is the first power norm of $r^{(k)}$; it is displayed at the end of each sweep through R_h . It is easily accumulated during the algorithm (15), since

$$||e_{\beta}^{(k)}|| = \sum_{R_k} |r_P^{(k)}|.$$

The ratio $||e_{\beta}^{(k)}||/||e_{\beta}^{(k-1)}||$ is also displayed, and is useful, for example, in approximating the σ of (17).

When R_h is a rectangle of 30 by 68 interior points, a relaxation sweep through the 2040 points takes SWAC 8.5 seconds. When $\beta=1$, to reduce $e_1^{(k)}$ by a factor of 10^{-6} would take about 2300 sweeps—over five hours on SWAC. Using the optimal value $\beta=\beta_0=1.858+$, only 90 sweeps would be needed—about 13 minutes on SWAC. Including the time necessary to estimate that 1.875 is a pretty good value for β , and running with this β , a reduction of 10^{-6} in $e_{\beta}^{(k)}$ is found in practice to take 20 or 30 minutes (see [15]).

Code 61 is a modification of Code 60 in which boundary conditions corresponding to $\partial u/\partial n = u_n = 0$ are permitted at any point of C_h . Suppose, for example, that it is desired to have $\partial u/\partial x = 0$ for x = 0, where R is a region with x > 0. Then values of u(x, y) for the lines x = -h, x = 0, x = h, x = 2h, \cdots are all stored on the drum for appropriate values of y. When the code comes to u(-h, y) for any y, the value is simply replaced by u(h, y). The values u(0, y), u(h, y), u(2h, y), \cdots are all relaxed according to (15). Again the relaxation routine is notified of the different types of interior and boundary points by suitable identification digits.

Mr. Kenneth Ralston of U.C.L.A. has prepared a SWAC code analogous to Code 60, dealing with curvilinear boundaries. Note in this case that it is no longer possible to map C_h onto the drum in a simple manner. For example, the point of C_h "north" of the point $(\mu h, \nu h)$ of R_h may not be the same as the point of C_h "west" of $(\mu h + h, \nu h + h)$. Identification digits distinguish: (a) points not in R_h , to be left alone, (b) regular interior points, to be treated by (15), with r_P as in (3), and (c) irregular interior points, to be treated by (15), with r_P as in (1).

To deal with irregular interior points Ralston stores the coefficients of u_E , u_W , u_N , u_S in formula (1) in four cells of certain special channels of the drum. Since one meets the irregular interior points of R_h in a fixed order, all these special coefficients can be stored once and for all in the proper sequence. (Such of the u_E , u_W , u_N , u_S as are fixed boundary values are actually multiplied into the coefficients stored in the special channels.) Ralston can also use the special channels to simulate a general mixed boundary condition $au_n + bu + c = 0$ on a straight boundary segment parallel to the x or y axis.

The author's Code 70 performs successive overrelaxation for the eigenvalue problem (6) over regions with no irregular interior points, following the method described in Section 3. The quantities β and $4-\lambda$ are both parameters of the code. Auxiliary to Code 70 are three other codes: Code 80 doubles the values of u over R_h , while Code 82 halves these values of u. Code 81 forms the Rayleigh quotient (20).

With Codes 70-82 the author found the fundamental eigenvalue for the L-shaped region of [3] for various h, and found the counter-example mentioned after (11). Code 61 has been adapted for some soil engineering calculations by Mr. D. Isherwood and Mrs. Louise Straus of U.C.L.A. Code 60 has been modified by Miss Rita Powers at U.C.L.A. to study the influence of the order in which the points of R_h are relaxed on the rate of convergence of successive overrelaxation.

To make Ralston's code more available for problems, a code is badly needed to tag the drum cells with the identification digits, to precompute the coefficients (1), and to store the latter on the special channels. Ralston and the author have outlined such a code, assuming C to be a piecewise quadratic function of x, y. Another needed code is one to get $\lambda_k^{(k)}$, for k > 1.

Using the ORACLE computer at Oak Ridge National Laboratories, W. C. Sangren [unpublished] has also computed $\lambda_h^{(1)}$ for the L-shaped region of [3] and for other simple regions with rectilinear boundaries.

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Received January 20, 1956.